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TDDFT Predictions of UV-vis Spectra in Ethanol for an Array of Curcumin Analogues

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TDDFT predictions of UV-vis spectra in ethanol for an array of curcumin analogues

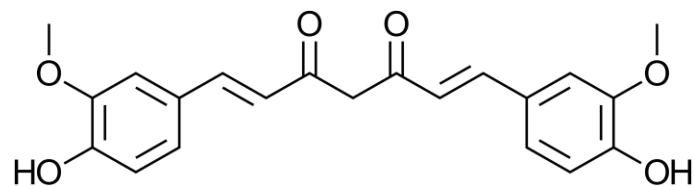


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Introduction

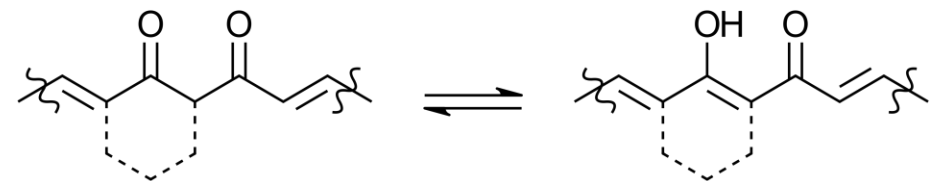


Curcumin is found in the common spice turmeric that can also be used as a dye and photosensitizer

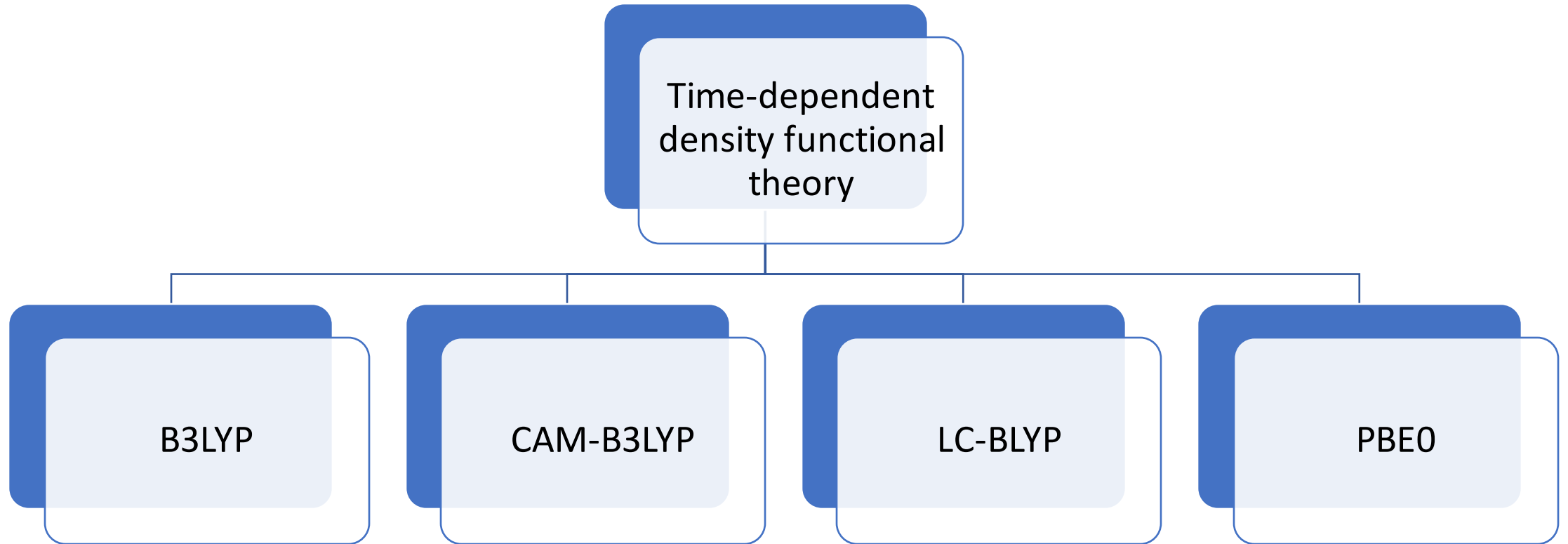


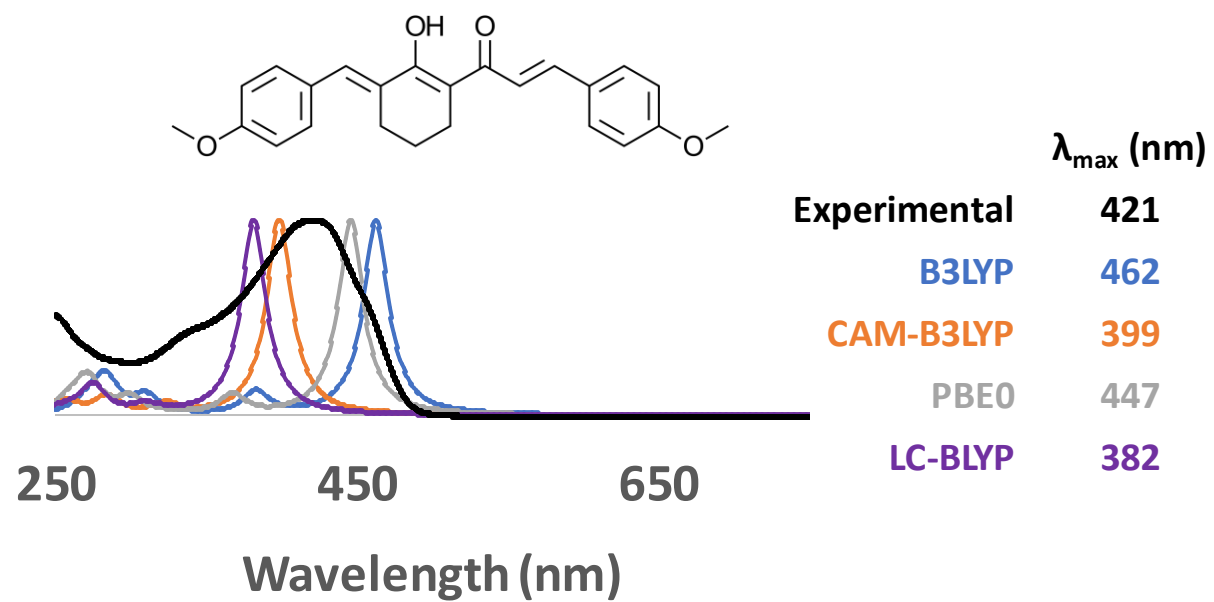
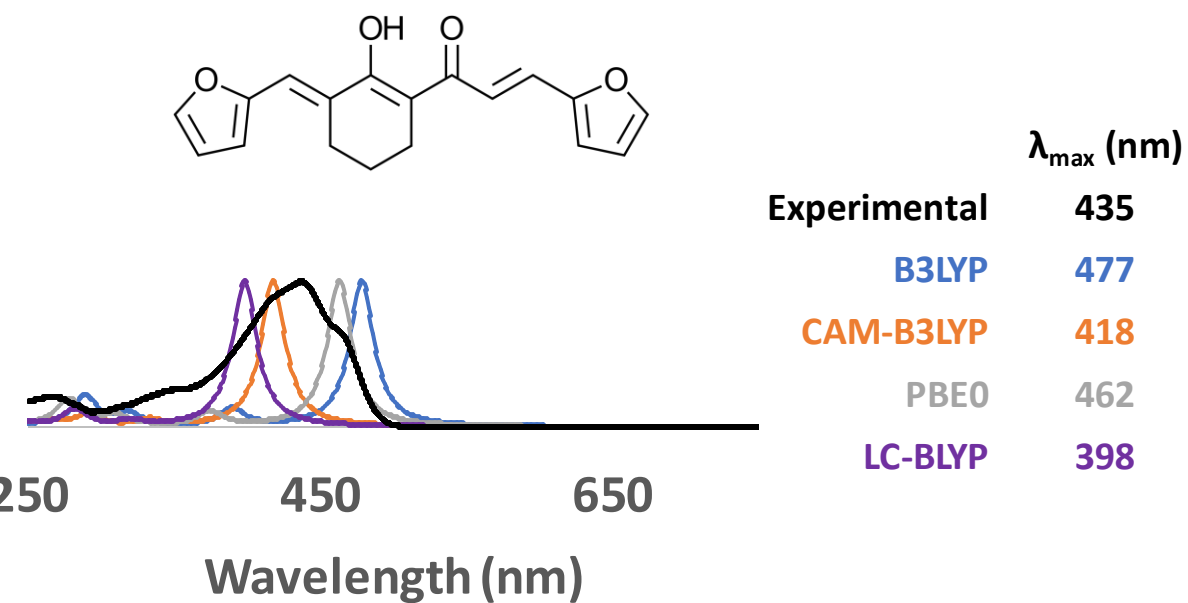
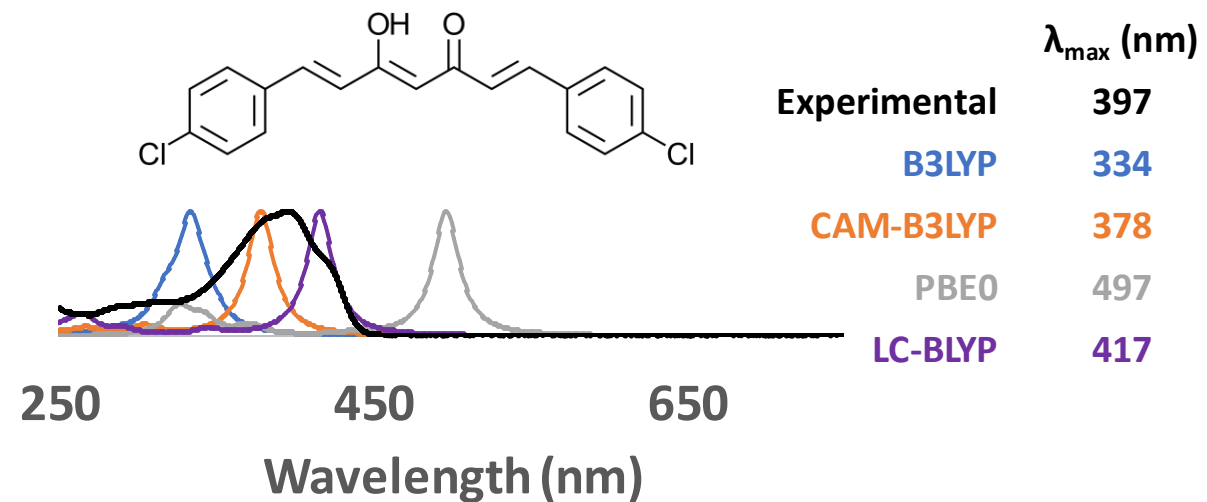
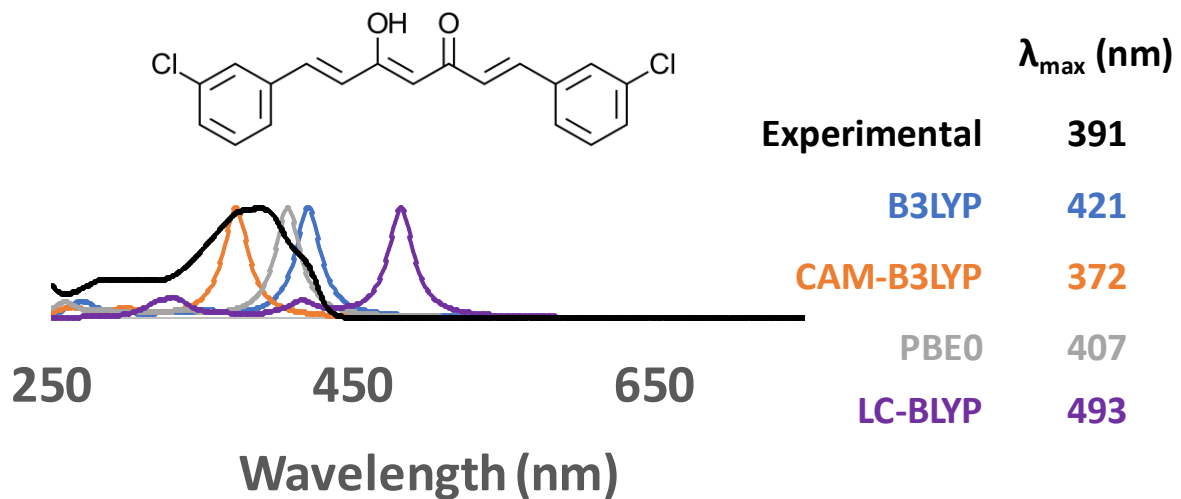
Accurately modeling UV-vis spectra can be challenging for extended conjugated systems

Curcuminoids undergo tautomerization – an exchange between two forms differing in the position of one H atom



Methods





Conclusions



- Generally, TDDFT methods can accurately predict λ_{max} values to within $\sim 10\text{--}12\%$ error
- CAM-B3LYP proved the most effective at reproducing UV-vis spectra (average error $< 5\%$)
- More curcuminoids will be modeled for comparisons to experimental UV-vis spectra and further validation of the CAM-B3LYP functional